Materials Science of Actinides
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Mission Statement: The mission of the Materials Science of Actinides (MSA) EFRC is to conduct transformative research in the actinide sciences with full integration of experimental and computational approaches, and an emphasis on research questions that are important to the energy future of the nation. Workforce development is a motivating goal of this university-based center.

The *Materials Science of Actinides* Center unites researchers from five universities and three national laboratories to conduct transformative research in actinide materials science. Actinides are, in many ways, at the frontier of exploration of the periodic table, as their chemistry is complicated by the importance of the 5*f* electrons, relativistic effects, and their complex redox chemistry. Owing to this complexity and the relative difficulty of working with actinides, research in actinide chemistry and actinide-based materials has lagged far behind that of most other elements in the periodic table, both in theory and synthesis and design for special properties, such as radiation resistance of actinide-bearing materials.

In actinides, the delocalization/localization of 5*f* electrons presents the possibility of control of materials processes at the level of electrons. Indeed these properties emerge from the complex correlations of atomic (composition and short and long-range order) and electronic (*f*-electron) constituents. In this center, we will heavily emphasize new synthesis approaches for actinide materials that are likely to lead to revolutionary new forms of matter with tailored properties. New materials that we emphasize are based upon the self-assembly of actinides into nanoscale materials with the potential to create new technologies. Radiation in actinide materials creates a system that is very far away from equilibrium, and a core focus of this center is to examine the behavior of actinide-based materials under extreme conditions of radiation, pressure and temperature.

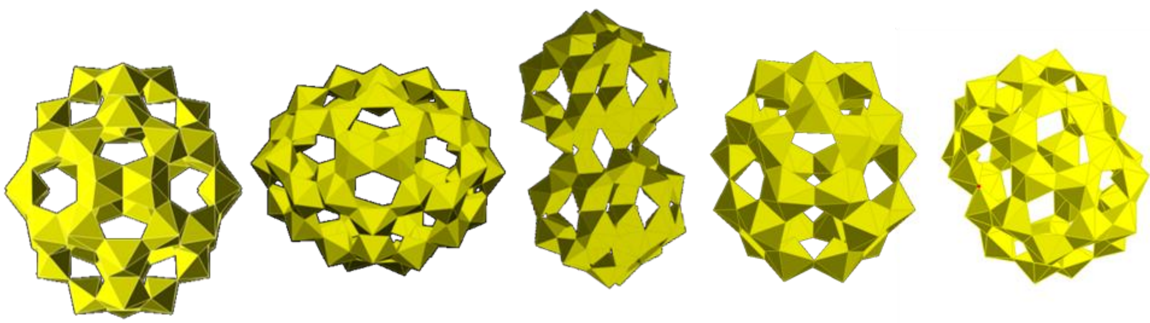
Three major Research Themes in actinide materials science are central to MSA's efforts. These themes are: Complex actinide materials, Nanoscale actinide materials, and Actinide materials under extreme environments. Four cross-cutting themes are: Actinide behavior at the nanoscale, Thermochemistry of actinide materials, Synthesis of new types of actinide materials, and Modeling of actinide materials.

The complex actinide materials theme includes the synthesis and properties of fluorite-structured materials with tetravalent actinides in solid solution, as well as the effects of extreme environments on such materials. It also encompasses the complex structural topologies typical of the higher-valence actinides, and details of the hydrothermal reactions used in synthesis of such materials.

The nanoscale actinide materials theme focuses on the self-assembly of actinide-centered polyhedra into complex clusters (see figure below). This research combines synthesis, synchrotron studies, computations, and thermodynamics to gain insights into the formation mechanisms, stability fields, and bonding requirements of such clusters.

The actinide materials under extreme environments theme examines the many phenomena in actinide solids that are temperature and/or pressure dependent – such as, order-disorder transformations, other phase transitions, and chemical decomposition. The coupling effects of extreme temperature and pressure environments with strong radiation fields are emphasized.

Our research will make essential use of DOE-BES and DOE-BER user facilities including, but not limited to, the Advanced Photon Source (APS) at Argonne National Laboratory (ANL), the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL), the Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory (PNNL), the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL), and the IVEM-Tandem Facility at ANL (as well as international facilities where comparable facilities do not exist in the U.S.).



Nanoscale uranyl peroxide clusters synthesized and structurally chracterized. Each cluster is built from uranyl hexagonal bipyramidal polyhedra. These clusters, which contain as many as 60 uranium atoms, self-assemble in alkaline solutions under ambient conditions.

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